



Electronic Device Simulation at the Classical-Quantum Transition Scale



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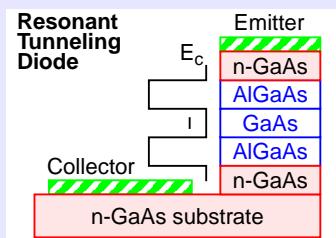


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Outline

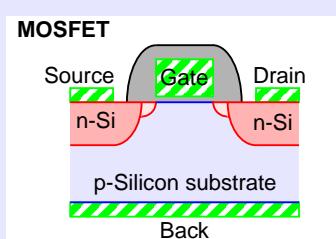
• Wigner Function Model

- Approach
- Results
- Plans



• Density-Gradient Model

- Approach
- Results
- Plans





Wigner Function Model (1D)



Wigner function transport equation (WFTE):

$$\frac{\partial f(x, k, t)}{\partial t} = - \underbrace{\frac{\hbar k}{m} \frac{\partial f}{\partial x}}_{\text{diffusion}} - \underbrace{\frac{1}{\hbar} \int \frac{dk'}{2\pi} V(x, k - k') f(x, k')}_{\text{drift}} + \underbrace{\left[\frac{\partial f}{\partial t} \right]_c}_{\text{scatter}}$$

$$V(x, k) \equiv \int [U(x+y) - U(x-y)] \sin[2yk] dy \quad \left. \frac{\partial f}{\partial t} \right|_c = \frac{\hbar}{\tau} \left(\frac{f_{\text{eq}}}{n_{\text{eq}}} n - f \right)$$

Poisson equation to enforce self-consistency:

$$\frac{\partial}{\partial x} \left[\epsilon(x) \frac{\partial u(x)}{\partial x} \right] = q\rho(x) = q^2 [C(x) - c(x)] \quad u(x) = U(x) - \delta U(x)$$

Charge and current density:

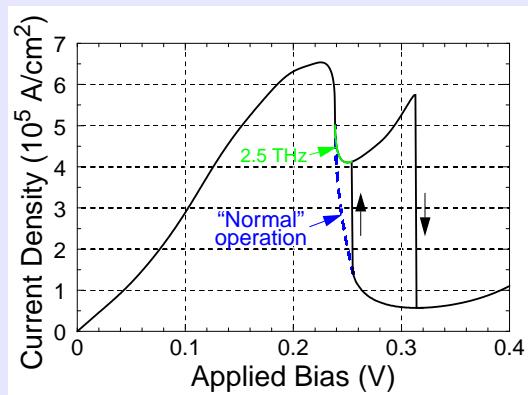
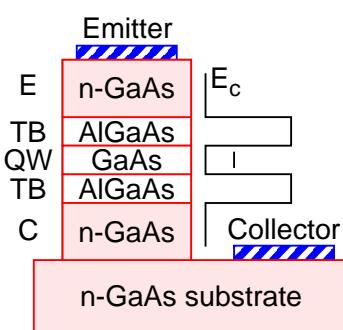
$$n(x, t) = \frac{1}{2\pi} \int f(x, k, t) dk \quad J(x, t) = \frac{1}{2\pi} \int \frac{\hbar k}{m} f(x, k, t) dk$$



Resonant Tunneling Diode Basics



Basic RTD Structure



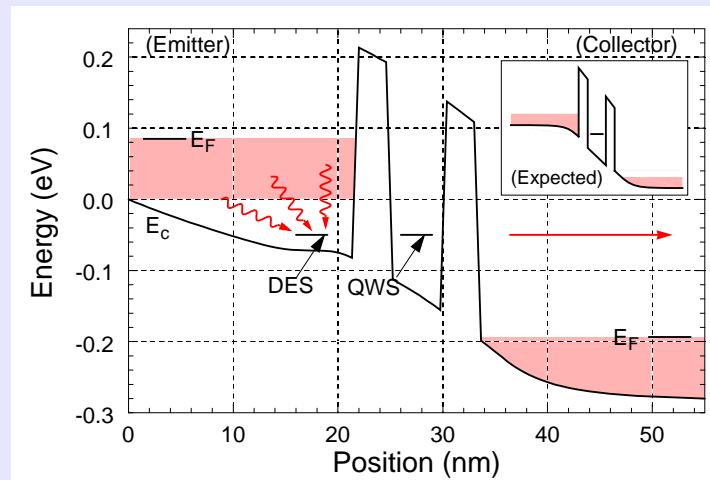
Novel simulated effects:

- Double current peak
- Steady-state hysteresis and bistability
- 2.5 THz oscillations at DC applied bias

Applications: 3-state/bistable device, microwave oscillator/detector



Second-Peak Current Path in RTD



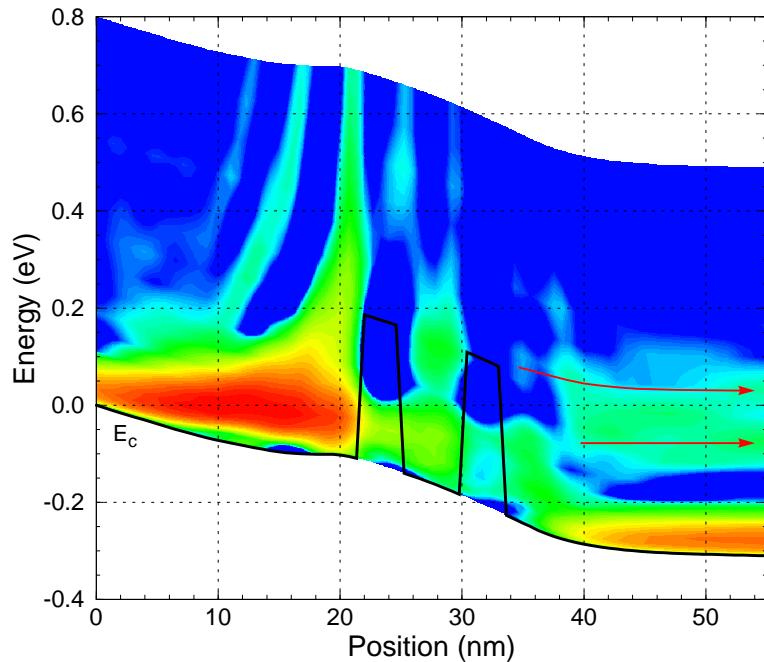
Second peak due to transmission through discrete emitter state (DES)

Bistability due to charge storage in QW

Oscillations due to NDR and variations in alignment of DES and QWS

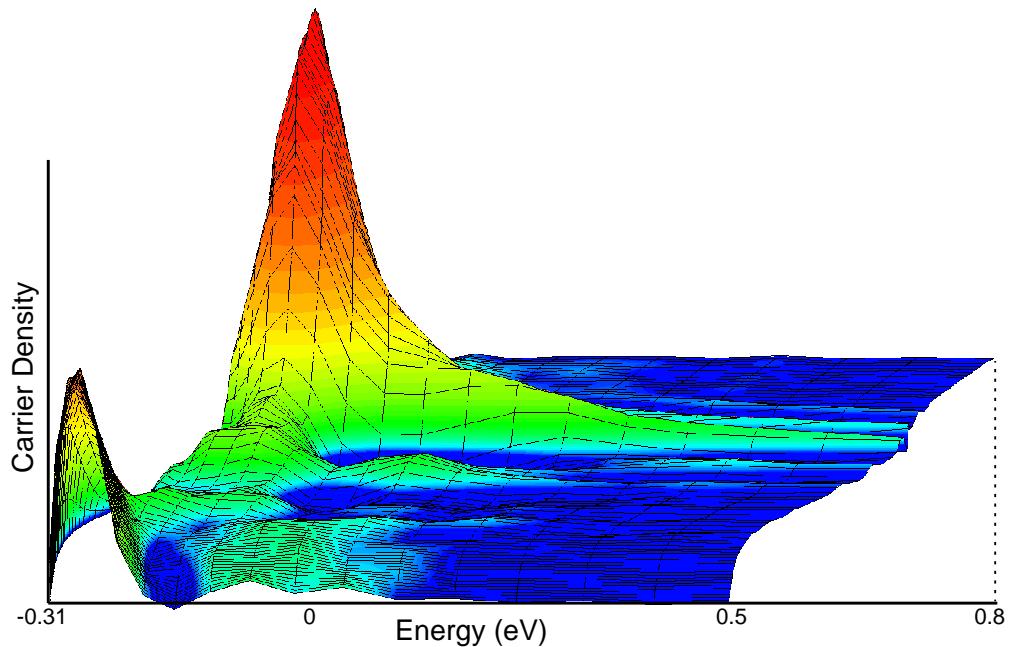


Carrier Density Contours (Plateau)

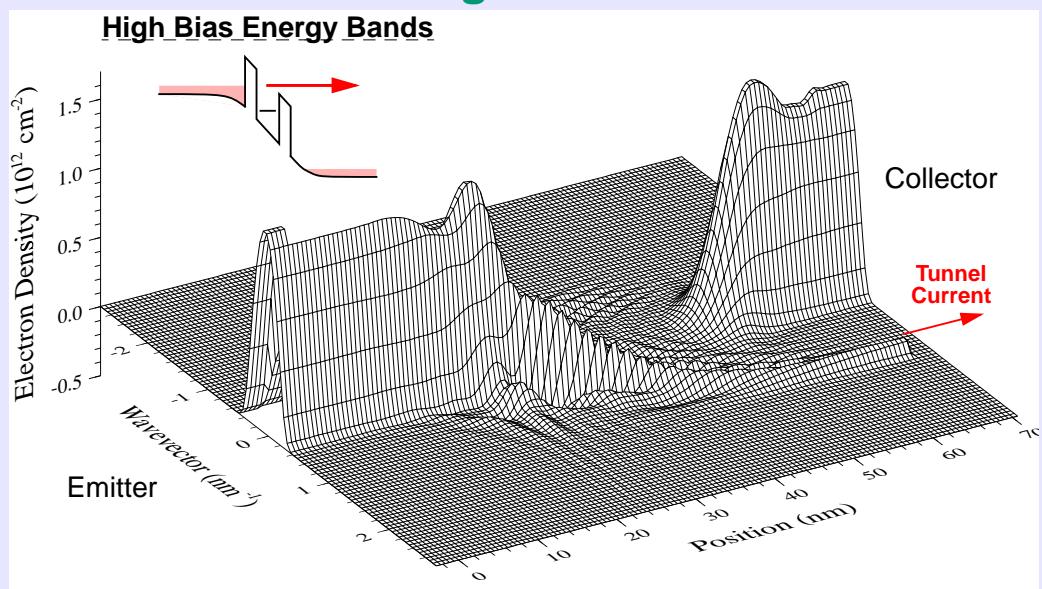




Carrier Density Contours (Plateau)



Wigner Function Example: RTD at High Bias





Strengths & Challenges of WF Model



Strengths:

- Classical: includes quantum effects
- Quantum: efficient scattering, ohmic BCs, transient simulation
- Related to BTE: experience
- WF is intuitively easy to interpret
- Direct interface to classical simulation regions

Challenges:

- Large matrix bandwidth: coarse momentum
- Non-uniform grids (position or momentum)
- Numerical error in drift term
- Classical contact (BC) model



Plans for Wigner Function Model



1-D Enhancements:

- Solve systematic error in standard implementation
- More accurate scattering models
- Non-uniform position and momentum grids
- Simulate tunneling devices, ultra-small MOSFETs in 1-D

Implementation of 2-D Capability:

- Migrate to PDE solver/parallel computation platform
- Iterative linear solver for huge computations
- Simulate ultra-small MOSFETs, quantum devices in 2-D



Density-Gradient Model



Density-Gradient Model (quantum-corrected drift-diffusion):

$$\frac{\partial n}{\partial t} = \nabla \cdot [D_n \nabla n - n \mu_n \nabla(u + u_{qn})]$$

$$u_{qn} \equiv 2b_n \left(\frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \right)$$

$$b_n \equiv \frac{-\hbar^2}{12m_n^* q}$$

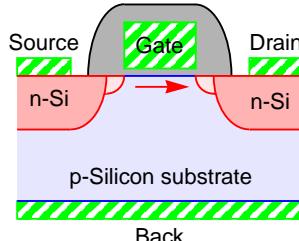
$$\frac{\partial p}{\partial t} = \nabla \cdot [D_p \nabla p + p \mu_p \nabla(u + u_{qp})]$$

$$u_{qp} \equiv -2b_p \left(\frac{\nabla^2 \sqrt{p}}{\sqrt{p}} \right)$$

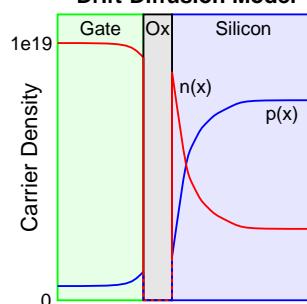
$$b_p \equiv \frac{\hbar^2}{12m_p^* q}$$

Effect of quantum potential:

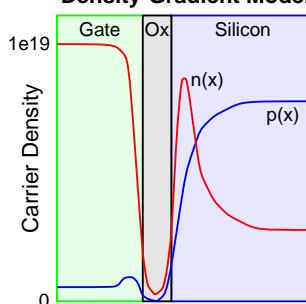
MOSFET Structure



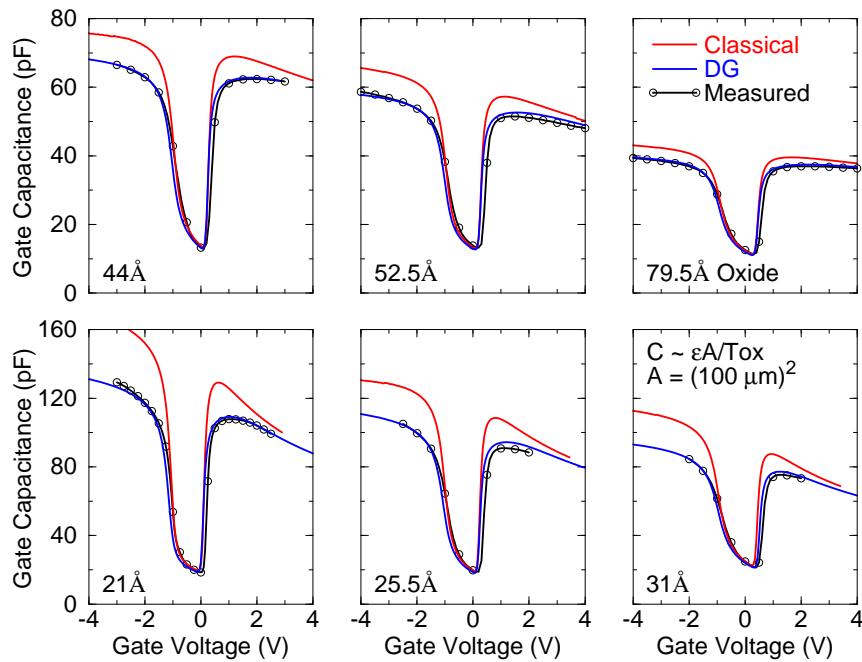
Drift-Diffusion Model



Density-Gradient Model

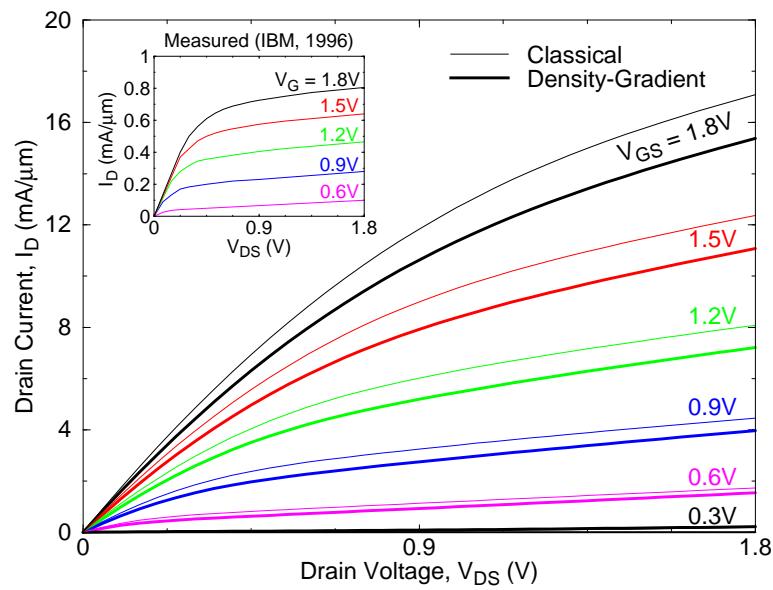


MOSFET C-V Simulation Results





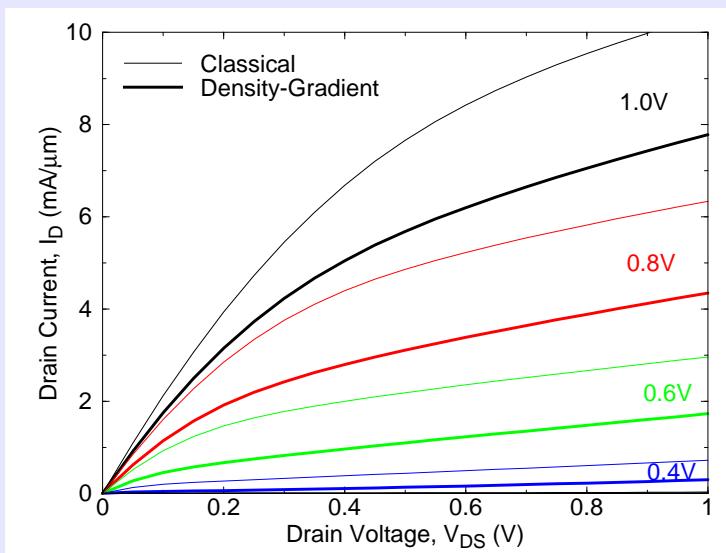
80 nm n-MOSFET Drain Characteristic



- Quantum effects reduce current by ~10%
- Mobility model and simulated structure need improvement!



30 nm n-MOSFET Drain Characteristic



Quantum-corrected current is 25% to 50% smaller



Strengths & Challenges of DG Model



Strengths:

- Similar to drift-diffusion model
- Relatively low cost for quantum effects
- 1-D, 2-D, 3-D transport, tunneling in unified model
- Implemented with PROPHET (PDE solver):
 - Rapid prototyping of, switching between, models
 - 1-D/2-D/3-D, structured/unstructured meshes
 - Modular structure for functionality upgrade

Challenges:

- Simple model of quantum effects and transport
- Current PROPHET limitations:
 - Anisotropic models (effective mass, mobility, ...)
 - Limited set of operators (e.g., no vector operators)
 - Non-intuitive user and developer interfaces



Plans for DG/PROPHET Project



Density-Gradient Model:

- Advanced mobility model (E-field, doping, surface dependence)
- Add heterostructure/tunneling capability to model
- 3-D transient simulations (e.g., SEU, switching)

PROPHET:

- Parallelization
- Anisotropic models (effective mass, mobility, ...)
- Advanced transport models (quantum hydro, BTE, WF, ...)
- Optoelectronic models
- Information Power Grid application
- Grand-challenge simulations